Propanoic acid, 2-(1-oxopropoxy)-, methyl ester

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 20.0 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.45e-01

Confidence level: 5.99e-01

Nearest Neighbors from the Training Set

Image not found	Image not found	Image not found
N-Methyl-N'-phenylurea	Urea, 1-(p-fluorophenyl)-	Urea, (3-methylphenyl)-
Measured: 19.5	**Measured:** 33.1	**Measured:** 36.3
Predicted: 29.8	**Predicted:** 49.6	**Predicted:** 37.2

Image not found	Image not found
1-Methoxy-2-propyl acetate	Urea, (m-fluorophenyl)-
Measured: 2.29	**Measured:** 58.9
Predicted: 7.33	**Predicted:** 59.1